

# Global $SO(3) \times SO(3) \times U(1)$ symmetry of the Hubbard model on bipartite lattices

J. M. P. Carmelo<sup>1</sup>, Stellan Östlund<sup>2</sup>, and M. J. Sampaio<sup>1</sup>

<sup>1</sup>*GCEP-Centre of Physics, University of Minho, Campus Gualtar, P-4710-057 Braga, Portugal and*

<sup>2</sup>*Göteborgs Universitet, Gothenburg 41296, Sweden*

(Dated: 22 August 2009)

In this paper the global symmetry of the Hubbard model on a bipartite lattice is found to be larger than  $SO(4)$ . The model is one of the most studied many-particle quantum problems, yet except in one dimension it has no exact solution, so that there remain many open questions about its properties. Symmetry plays an important role in physics and often can be used to extract useful information on unsolved non-perturbative quantum problems. Specifically, here it is found that for on-site interaction  $U \neq 0$  the local  $SU(2) \times SU(2) \times U(1)$  gauge symmetry of the Hubbard model on a bipartite lattice with  $N_a^D$  sites and vanishing transfer integral  $t = 0$  can be lifted to a global  $[SU(2) \times SU(2) \times U(1)]/Z_2^2 = SO(3) \times SO(3) \times U(1)$  symmetry in the presence of the kinetic-energy hopping term of the Hamiltonian with  $t > 0$ . (Examples of a bipartite lattice are the  $D$ -dimensional cubic lattices of lattice constant  $a$  and edge length  $L = N_a a$  for which  $D = 1, 2, 3, \dots$  in the number  $N_a^D$  of sites.) The generator of the new found hidden independent charge global  $U(1)$  symmetry, which is not related to the ordinary  $U(1)$  gauge subgroup of electromagnetism, is one half the rotated-electron number of singly-occupied sites operator. Although addition of chemical-potential and magnetic-field operator terms to the model Hamiltonian lowers its symmetry, such terms commute with it. Therefore, its  $4^{N_a^D}$  energy eigenstates refer to representations of the new found global  $[SU(2) \times SU(2) \times U(1)]/Z_2^2 = SO(3) \times SO(3) \times U(1)$  symmetry. Consistently, we find that for the Hubbard model on a bipartite lattice the number of independent representations of the group  $SO(3) \times SO(3) \times U(1)$  equals the Hilbert-space dimension  $4^{N_a^D}$ . It is confirmed elsewhere that the new found symmetry has important physical consequences.

PACS numbers: 02.20.Qs, 71.10.Fd

## I. INTRODUCTION

The Hubbard model on a bipartite lattice (for instance one-dimensional, square, cubic, and other  $D$ -dimensional cubic lattices) is the simplest realistic toy model for description of the electronic correlation effects in general many-particle problems with short-range interaction. It can be experimentally realized with unprecedented precision in systems of ultra-cold fermionic atoms on an optical lattice of variable geometry. For the square and cubic lattices one may expect very detailed experimental results over a wide range of parameters to be available<sup>1</sup>. For instance, recently systems of ultra-cold fermionic atoms describing the Mott-Hubbard insulating phase of the the Hubbard model on a cubic lattice were studied<sup>2</sup>. On the one dimensional and square lattices the model has been widely used for describing the effects of correlations in several types of materials such as quasi-one-dimensional conductors<sup>3,4</sup> and high- $T_c$  superconductors<sup>5-7</sup>.

Unfortunately, most exact results and well-controlled approximations for this model exist only in one dimension (1D)<sup>8-10</sup>. Many open questions about its properties remain unsolved. One of the few exact results, which refers to the model on any bipartite lattice, is that for on-site interaction  $U \neq 0$  it contains a global  $SO(4) = [SU(2) \times SU(2)]/Z_2$  symmetry. It is associated with a spin  $SU(2)$  symmetry and a charge  $\eta$ -spin  $SU(2)$  symmetry<sup>11</sup>. We denote the  $\eta$ -spin (and spin) value of the energy eigenstates by  $S_\eta$  (and  $S_s$ ) and the corresponding projection by  $S_\eta^z = -[N_a^D - N]/2$  (and  $S_s^z = -[N_\uparrow - N_\downarrow]/2$ ). Here  $N_a^D$  denotes the number of lattice sites and  $N = N_\uparrow + N_\downarrow$  that of electrons. Our notation  $N_a^D$  is particularly appropriate to a  $D$ -dimensional cubic lattice where  $D = 1, 2, 3, \dots$  for the one-dimensional, square, cubic ... lattice, respectively,  $N_a$  is the number of sites in an edge of length  $L = N_a a$ , and  $a$  is the spacing.

In this paper we find that for  $U \neq 0$  the local  $SU(2) \times SU(2) \times U(1)$  gauge symmetry of the Hubbard model on a bipartite lattice with transfer integral  $t = 0$ <sup>12</sup> can be lifted to a global  $[SU(2) \times SU(2) \times U(1)]/Z_2^2 = SO(3) \times SO(3) \times U(1)$  symmetry for the model with  $t > 0$ . Indeed, the requirement of commutability with the  $U/4t \neq 0$  interacting Hamiltonian replaces the  $U = 0$  global  $O(4)/Z_2 = [SO(4) \times Z_2]/Z_2$  symmetry by  $SO(3) \times SO(3) \times U(1) = [SO(4) \times U(1)]/Z_2$  rather than  $SO(4)$ . Here, the factor  $Z_2$  in  $SO(4) \times Z_2$  refers to the particle-hole transformation on a single spin under which the interacting term is not invariant<sup>12</sup>. In  $O(4)/Z_2$  and  $[SU(2) \times SU(2) \times U(1)]/Z_2^2 = SO(3) \times SO(3) \times U(1)$  the factors  $1/Z_2$  and  $1/Z_2^2$  impose that  $[S_\eta + S_s]$  and  $[S_\eta + S_s + S_c]$ , respectively, are integers. In the latter equations  $S_c$  is the eigenvalue of the generator of the new global  $U(1)$  symmetry found in this paper. Our results profit from those of Ref.<sup>13</sup> and reveal that such a symmetry becomes explicit, provided that one describes the problem in terms of rotated electrons. Those are generated by any of the unitary transformations considered in that reference, which refer to  $U/4t > 0$  values and can be trivially extended to  $U/4t \neq 0$  values. The global symmetry

found here refers to the latter  $U/4t$  range.

The paper is organized as follows. The model and the electron - rotated-electron unitary transformations are the subjects of Section II. In Section III a global  $SO(3) \times SO(3) \times U(1)$  symmetry is established for the Hubbard model on a bipartite lattice with  $U/4t \neq 0$ . Finally, Section IV contains the concluding remarks.

## II. THE MODEL AND A SET USEFUL ELECTRON - ROTATED-ELECTRON UNITARY TRANSFORMATIONS

On a bipartite lattice with spacing  $a$ ,  $N_a^D \equiv [N_a]^D$  sites,  $N_a$  even,  $N_a/2$  odd,  $L = N_a a$ , and spatial dimension  $D < N_a$  the Hubbard model is given by,

$$\hat{H} = \hat{T} + \frac{U}{2}[N_a^D - \hat{Q}]; \quad \hat{T} = -t \sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma=\uparrow, \downarrow} [c_{\vec{r}_j, \sigma}^\dagger c_{\vec{r}_{j'}, \sigma} + h.c.]; \quad \hat{Q} = \sum_{j=1}^{N_a^D} \sum_{\sigma=\uparrow, \downarrow} \hat{n}_{\vec{r}_j, \sigma} (1 - \hat{n}_{\vec{r}_j, -\sigma}). \quad (1)$$

Here  $\hat{T}$  is the kinetic-energy operator with first-neighbor transfer integral  $t$ , which can be expressed in terms of the operators,

$$\begin{aligned} \hat{T}_0 &= - \sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma} [\hat{n}_{\vec{r}_j, -\sigma} c_{\vec{r}_j, \sigma}^\dagger c_{\vec{r}_{j'}, \sigma} \hat{n}_{\vec{r}_{j'}, -\sigma} + (1 - \hat{n}_{\vec{r}_j, -\sigma}) c_{\vec{r}_j, \sigma}^\dagger c_{\vec{r}_{j'}, \sigma} (1 - \hat{n}_{\vec{r}_{j'}, -\sigma}) + h.c.], \\ \hat{T}_{+1} &= - \sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma} \hat{n}_{\vec{r}_j, -\sigma} c_{\vec{r}_j, \sigma}^\dagger c_{\vec{r}_{j'}, \sigma} (1 - \hat{n}_{\vec{r}_{j'}, -\sigma}), \\ \hat{T}_{-1} &= - \sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma} (1 - \hat{n}_{\vec{r}_j, -\sigma}) c_{\vec{r}_j, \sigma}^\dagger c_{\vec{r}_{j'}, \sigma} \hat{n}_{\vec{r}_{j'}, -\sigma}, \end{aligned} \quad (2)$$

as  $\hat{T} = t[\hat{T}_0 + \hat{T}_{+1} + \hat{T}_{-1}]$ . While the operator  $\hat{T}_0$  does not change electron double occupancy, the operators  $\hat{T}_{+1}$  and  $\hat{T}_{-1}$  do it by  $+1$  and  $-1$ , respectively. In the above equations  $\hat{n}_{\vec{r}_j, \sigma} = c_{\vec{r}_j, \sigma}^\dagger c_{\vec{r}_j, \sigma}$ ,  $\pm\sigma$  refer to opposite spin projections, and the operator  $\hat{Q}$  counts the number of electron singly occupied sites. Hence the operators,

$$\hat{D} = \frac{1}{2}[\hat{N} - \hat{Q}]; \quad \hat{D}^h = \frac{1}{2}[\hat{N}^h - \hat{Q}]; \quad \hat{Q}_\uparrow = \frac{1}{2}[\hat{Q} + (\hat{N}_\uparrow - \hat{N}_\downarrow)]; \quad \hat{Q}_\downarrow = \frac{1}{2}[\hat{Q} - (\hat{N}_\uparrow - \hat{N}_\downarrow)], \quad (3)$$

count the number of electron doubly occupied sites, unoccupied sites, and spin  $\sigma = \uparrow, \downarrow$  singly occupied sites, respectively. Moreover,  $\hat{N} = \sum_{\sigma} \hat{N}_\sigma$  and  $\hat{N}_\sigma = \sum_{j=1}^{N_a^D} n_{\vec{r}_j, \sigma}$  where  $\hat{N}^h = [2N_a^D - \hat{N}]$ ,  $\hat{N}_\uparrow^h = [N_a^D - \hat{N}_\downarrow]$ , and  $\hat{N}_\downarrow^h = [N_a^D - \hat{N}_\uparrow]$ .

For simplicity let us consider that  $U/4t > 0$  and let  $\{|\Psi_\infty\rangle\}$  be a complete set of  $4^{N_a^D}$  energy eigenstates for  $U/4t \rightarrow \infty$ . There is exactly one unitary operator  $\hat{V} = \hat{V}(U/4t)$  such that for the value of  $U/4t > 0$  under consideration each of the  $4^{N_a^D}$  states  $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle$  is generated from the electronic vacuum by the same occupancy configurations of *rotated electrons* of creation operator  $\tilde{c}_{\vec{r}_j, \sigma}^\dagger$  as the corresponding  $U/4t \rightarrow \infty$  energy eigenstate in terms of electrons. The rotated-electron creation and annihilation operators are given by,

$$\tilde{c}_{\vec{r}_j, \sigma}^\dagger = \hat{V}^\dagger c_{\vec{r}_j, \sigma}^\dagger \hat{V}; \quad \tilde{c}_{\vec{r}_j, \sigma} = \hat{V}^\dagger c_{\vec{r}_j, \sigma} \hat{V}; \quad \tilde{n}_{\vec{r}_j, \sigma} = \tilde{c}_{\vec{r}_j, \sigma}^\dagger \tilde{c}_{\vec{r}_j, \sigma}. \quad (4)$$

Rotated-electron single and double occupancy are good quantum numbers for  $U/4t > 0$  whereas for electrons such occupancies become good quantum numbers only for  $U/4t \rightarrow \infty$ . Therefore,  $\hat{V} = \hat{V}(U/4t)$  becomes the unit operator in that limit. The unitary transformation associated with the operator  $\hat{V}$  is of the type studied in Ref.<sup>13</sup>. There is one of such transformations for each choice of  $U/4t \rightarrow \infty$  energy eigenstates. Similar results are obtained for  $U/4t < 0$ .

We introduce the operator  $\tilde{O} = \hat{V}^\dagger \hat{O} \hat{V}$ . It has the same expression in terms of rotated-electron creation and annihilation operators as  $\hat{O}$  in terms of electron creation and annihilation operators. Here  $\hat{V} = \tilde{V}$ . Note that within our representation both the notations referring to marks placed over letters being a caret  $\hat{W}$  or a tilde  $\tilde{L}$  denote operators. Such notations are useful for operators for which  $W = L$  such as the general operators  $\hat{O}$  and  $\tilde{O}$ . Indeed, then they imply the equivalent relations  $\tilde{O} = \hat{V}^\dagger \hat{O} \hat{V}$  and  $\hat{O} = \tilde{V} \tilde{O} \tilde{V}^\dagger$ . (Here we have used that  $\hat{V} = \tilde{V}$ .) When  $\hat{O} \neq \tilde{O}$  our convention is that in general the expression of the operator  $\hat{O}$  in terms of electron creation and annihilation operators is simpler than that of  $\tilde{O} = \hat{V}^\dagger \hat{O} \hat{V}$  in terms such operators. This then implies that the expression of  $\tilde{O}$  in terms of rotated-electron creation and annihilation operators is simpler than that of  $\hat{O} = \tilde{V} \tilde{O} \tilde{V}^\dagger$  in terms of the

same rotated-electron operators. (An exception are the electron operators of Eq. (4), which denote by  $c_{\vec{r}_j,\sigma}^\dagger$  and  $c_{\vec{r}_j,\sigma}$  rather than by  $\hat{c}_{\vec{r}_j,\sigma}^\dagger$  and  $\hat{c}_{\vec{r}_j,\sigma}$ , respectively.)

Any operator  $\hat{O}$  can be written as,

$$\hat{O} = \hat{V} \tilde{O} \hat{V}^\dagger = \tilde{O} + [\tilde{O}, \hat{S}] + \frac{1}{2} [[\tilde{O}, \hat{S}], \hat{S}] + \dots = \tilde{V} \tilde{O} \tilde{V}^\dagger = \tilde{O} + [\tilde{O}, \tilde{S}] + \frac{1}{2} [[\tilde{O}, \tilde{S}], \tilde{S}] + \dots, \quad (5)$$

where  $\hat{V}^\dagger = e^{\hat{S}}$ ,  $\hat{V} = e^{-\hat{S}}$ , and  $\hat{S} = \tilde{S}$ . That  $\hat{S}$  and  $\hat{V}$  have the same expression both in terms of electron and rotated-electron creation and annihilation operators justifies that  $\hat{O} = \hat{V} \tilde{O} \hat{V}^\dagger = \tilde{V} \tilde{O} \tilde{V}^\dagger$  in Eq. (5). Importantly, it follows from the results of Ref.<sup>13</sup> that for each electron - rotated-electron unitary transformation and corresponding unitary operator  $\hat{V}$  of the type considered in that reference the operator  $\hat{S}$  has a uniquely defined expression. For any of such transformations that unknown expression of  $\hat{S}$  involves only the kinetic operators  $\hat{T}_0$ ,  $\hat{T}_{+1}$ , and  $\hat{T}_{-1}$  of Eq. (2) and numerical  $U/4t$  dependent coefficients. For  $U/4t \neq 0$  it can be expanded in a series of  $t/U$ . Importantly, the corresponding first-order term has a universal form for all electron - rotated-electron unitary transformations of the above-mentioned type, which reads<sup>13</sup>,

$$\hat{S} = -\frac{t}{U} [\hat{T}_{+1} - \hat{T}_{-1}] + \mathcal{O}(t^2/U^2) = \tilde{S} = -\frac{t}{U} [\tilde{T}_{+1} - \tilde{T}_{-1}] + \mathcal{O}(t^2/U^2). \quad (6)$$

(The form of our relation  $\hat{V}^\dagger = e^{\hat{S}}$  justifies the extra minus sign in the  $\hat{S}$  and  $\tilde{S}$  expressions given here, relative to those of Ref.<sup>13</sup>.)

Furthermore, for any unitary operator  $\hat{V}$  of the above type,  $-\hat{S}$  can be written as  $-\hat{S} = \hat{S}(\infty) + \Delta\hat{S}$ . Here  $\hat{S}(\infty)$  corresponds to the operator  $S(l)$  for  $l = \infty$  defined in Eq. (61) of Ref.<sup>13</sup> and  $\Delta\hat{S}$  has the general form provided in Eq. (64) of that reference. For each specific transformation and corresponding choice of  $U/4t \rightarrow \infty$  energy eigenstates there is exactly one choice for the numbers  $D^{(k)}(\mathbf{m})$  in that equation. ( $k = 1, 2, \dots$  refers to the number of rotated-electron doubly occupied sites.)

Since  $\hat{V}$  is unitary, the operators  $\hat{c}_{\vec{r}_j,\sigma}^\dagger$  and  $\tilde{c}_{\vec{r}_j,\sigma}$  have the same anticommutation relations as  $c_{\vec{r}_j,\sigma}^\dagger$  and  $c_{\vec{r}_j,\sigma}$ . The  $\sigma$  electron number operator  $\hat{N}_\sigma = \sum_{j=1}^{N_a^D} \hat{n}_{\vec{r}_j,\sigma}$  equals the corresponding  $\sigma$  rotated-electron number operator  $\tilde{N}_\sigma = \sum_{j=1}^{N_a^D} \tilde{n}_{\vec{r}_j,\sigma}$ . As a result, it remains invariant under  $\hat{V}$ , so that  $[\hat{N}_\sigma, \hat{V}] = [\hat{N}_\sigma, \hat{S}] = 0$ . (See equation (5) such that  $[\tilde{N}_\sigma, \tilde{S}] = 0$  for  $\hat{O} = \hat{N}_\sigma$  and  $\tilde{O} = \tilde{N}_\sigma$ .)

### III. THE GLOBAL $SO(3) \times SO(3) \times U(1)$ SYMMETRY FOR $U/4t \neq 0$

#### A. Global symmetry of the Hubbard model on a general bipartite lattice

The local  $SU(2) \times SU(2) \times U(1)$  gauge symmetry of the Hamiltonian (1) for  $U/4t \rightarrow \pm\infty$  considered in Ref.<sup>12</sup> becomes for finite  $|U/4t| > 0$  values a group of permissible unitary transformations. It is such that the corresponding local  $U(1)$  canonical transformation is not the ordinary  $U(1)$  gauge subgroup of electromagnetism. Instead it is a “nonlinear” transformation<sup>12</sup>. Following the unitary character of  $\hat{V} = \tilde{V}$ , one can either consider that,

$$\hat{H} = \hat{V} \tilde{H} \hat{V}^\dagger = \tilde{V} \tilde{H} \tilde{V}^\dagger = \tilde{H} + [\tilde{H}, \tilde{S}] + \frac{1}{2} [[\tilde{H}, \tilde{S}], \tilde{S}] + \dots, \quad (7)$$

is the Hubbard model written in terms of rotated-electron operators or another Hamiltonian with an involved expression and whose operators  $\tilde{c}_{\vec{r}_j,\sigma}^\dagger$  and  $\tilde{c}_{\vec{r}_j,\sigma}$  refer to electrons. According to Ref.<sup>13</sup>, the latter rotated Hamiltonian is built up by use of the conservation of singly occupancy  $2S_c = \langle \tilde{Q} \rangle$  by eliminating terms in the  $t > 0$  Hubbard Hamiltonian. That is done so that  $S_c$  is an eigenvalue of the following one-half rotated-electron singly-occupancy number operator associated with the operator  $\tilde{S}_c \equiv \tilde{Q}/2$ ,

$$\tilde{S}_c \equiv \frac{1}{2} \hat{V}^\dagger \hat{Q} \hat{V} = \frac{1}{2} \tilde{Q} = \frac{1}{2} \sum_{j=1}^{N_a^D} \sum_{\sigma=\uparrow,\downarrow} \tilde{n}_{\vec{r}_j,\sigma} (1 - \tilde{n}_{\vec{r}_j,-\sigma}). \quad (8)$$

Here  $\tilde{n}_{\vec{r}_j,\sigma} = \hat{V}^\dagger \hat{n}_{\vec{r}_j,\sigma} \hat{V} = \tilde{c}_{\vec{r}_j,\sigma}^\dagger \tilde{c}_{\vec{r}_j,\sigma}$  is the operator given in Eq. (4). According to the studies of Ref.<sup>13</sup>, this can be done to all orders of  $t/U$  provided that  $U/4t \neq 0$ . In the context of Ref.<sup>14</sup>, this is equivalent to compute rotated “quasicharge” fermions whose number exactly equals  $[N_a^D - 2S_c]$ .

The “rotated” Hamiltonian  $\tilde{H} = \hat{V}^\dagger \hat{H} \hat{V}$  commutes with the six generators of the  $SO(4)$  symmetry. Thus the Hubbard model  $\hat{H}$  commutes with both such generators and corresponding six other operators with the same expressions when written in terms of rotated-electron operators. Consistently with Eq. (5), this just means that the six generators of the  $\eta$ -spin and spin algebras commute with  $\hat{V}$ . To reach this result we have profited from the expression of the operator  $\hat{S}$  only involving the three kinetic operators given in Eq. (2). We have then calculated the following commutators,

$$[\hat{S}_\alpha^z, \hat{T}_l] = [\hat{S}_\alpha^\dagger, \hat{T}_l] = [\hat{S}_\alpha, \hat{T}_l] = 0; \quad \alpha = \eta, s, \quad l = 0, \pm 1. \quad (9)$$

Although the algebra involved in their derivation is cumbersome, it is straightforward. Therefore, we omit here the corresponding details. The vanishing of the commutators (9) implies that the six generators of the  $\eta$ -spin and spin algebras commute with  $\hat{V}$ ,

$$[\hat{S}_\alpha^z, \hat{V}] = [\hat{S}_\alpha^\dagger, \hat{V}] = [\hat{S}_\alpha, \hat{V}] = 0; \quad \alpha = \eta, s. \quad (10)$$

This confirms that for such six operators all operator terms on the right-hand side of Eq. (5) containing commutators vanish so that  $\hat{O} = \tilde{O}$  for  $\hat{O}$  being any of such operators. Hence they have the same expression in terms of electron and rotated-electron operators and read,

$$\begin{aligned} \hat{S}_\eta^z &= -\frac{1}{2}[N_a^D - \hat{N}] = -\frac{1}{2}[N_a^D - \tilde{N}]; \quad \hat{S}_s^z = -\frac{1}{2}[\hat{N}_\uparrow - \hat{N}_\downarrow] = -\frac{1}{2}[\tilde{N}_\uparrow - \tilde{N}_\downarrow], \\ \hat{S}_\eta^\dagger &= \sum_{j=1}^{N_a^D} e^{i\vec{\pi} \cdot \vec{r}_j} c_{\vec{r}_j \downarrow}^\dagger c_{\vec{r}_j \uparrow} = \sum_{j=1}^{N_a^D} e^{i\vec{\pi} \cdot \vec{r}_j} \tilde{c}_{\vec{r}_j \downarrow}^\dagger \tilde{c}_{\vec{r}_j \uparrow}^\dagger; \quad \hat{S}_\eta = \sum_{j=1}^{N_a^D} e^{-i\vec{\pi} \cdot \vec{r}_j} c_{\vec{r}_j \uparrow} c_{\vec{r}_j \downarrow} = \sum_{j=1}^{N_a^D} e^{-i\vec{\pi} \cdot \vec{r}_j} \tilde{c}_{\vec{r}_j \uparrow} \tilde{c}_{\vec{r}_j \downarrow}, \\ \hat{S}_s^\dagger &= \sum_{j=1}^{N_a^D} c_{\vec{r}_j \downarrow}^\dagger c_{\vec{r}_j \uparrow} = \sum_{j=1}^{N_a^D} \tilde{c}_{\vec{r}_j \downarrow}^\dagger \tilde{c}_{\vec{r}_j \uparrow}; \quad \hat{S}_s = \sum_{j=1}^{N_a^D} c_{\vec{r}_j \uparrow} c_{\vec{r}_j \downarrow} = \sum_{j=1}^{N_a^D} \tilde{c}_{\vec{r}_j \uparrow} \tilde{c}_{\vec{r}_j \downarrow}, \end{aligned} \quad (11)$$

where the vector  $\vec{\pi}$  has Cartesian components  $\vec{\pi} = [\pi, \pi, \dots]$ . For instance, for the model on the 1D, square, and cubic lattices those read  $\pi$ ,  $[\pi, \pi]$ , and  $[\pi, \pi, \pi]$ , respectively.

In addition, we have evaluated the commutators of the three components of the momentum operator  $\hat{\vec{P}}$  with the three operators of Eq. (2). Again all such commutators vanish, so that the momentum operator commutes with  $\hat{V}$ . Use of Eq. (5) then implies that such an operator reads,

$$\hat{\vec{P}} = \sum_{\sigma=\uparrow, \downarrow} \sum_{\vec{k}} \vec{k} c_{\vec{k}, \sigma}^\dagger c_{\vec{k}, \sigma} = \sum_{\sigma=\uparrow, \downarrow} \sum_{\vec{k}} \vec{k} \tilde{c}_{\vec{k}, \sigma}^\dagger \tilde{c}_{\vec{k}, \sigma}. \quad (12)$$

Again all operator terms on the right-hand side of Eq. (5) containing commutators vanish for  $\hat{O}$  being any of the three operator components of  $\hat{\vec{P}}$ , so that  $\hat{\vec{P}} = \tilde{\vec{P}}$ .

According to the studies of Ref.<sup>12</sup>, the  $SU(2) \times SU(2) \times U(1)$  Lie group and its local generators can be represented by the  $4 \times 4$  on-site matrix  $x_{\vec{r}_j}$  provided in Eq. (7) of that reference and matrices  $o_{\vec{r}_j}$  appropriate to these generators. Their entries are given through polynomials of electron operators of the general form  $\hat{X}_{\vec{r}_j} = \sum_{l, l'} x_{\vec{r}_j, l, l'} \hat{m}_{\vec{r}_j, l, l'} \equiv \text{Tr}(x_{\vec{r}_j} \hat{m}_{\vec{r}_j})$  and  $\hat{O}_{\vec{r}_j} = \sum_{l, l'} o_{\vec{r}_j, l, l'} \hat{m}_{\vec{r}_j, l, l'} \equiv \text{Tr}(o_{\vec{r}_j} \hat{m}_{\vec{r}_j})$ , respectively. Here the operator matrix  $\hat{m}_{\vec{r}_j}$  has the same form as the operator matrix  $\tilde{m}_{\vec{r}_j} = \hat{V}^\dagger \hat{m}_{\vec{r}_j} \hat{V}$ , but with the rotated-electron operators replaced by electron operators. The operator matrix  $\tilde{m}_{\vec{r}_j}$  plays an important role in our studies. It reads,

$$\tilde{m}_{\vec{r}_j} = \begin{bmatrix} 1 - \tilde{n}_{\vec{r}_j, \uparrow} - \tilde{n}_{\vec{r}_j, \downarrow} + \tilde{n}_{\vec{r}_j, \uparrow} \tilde{n}_{\vec{r}_j, \downarrow} & \tilde{c}_{\vec{r}_j, \downarrow} \tilde{c}_{\vec{r}_j, \uparrow} & (1 - \tilde{n}_{\vec{r}_j, \downarrow}) \tilde{c}_{\vec{r}_j, \uparrow} & (1 - \tilde{n}_{\vec{r}_j, \uparrow}) \tilde{c}_{\vec{r}_j, \downarrow} \\ \tilde{c}_{\vec{r}_j, \uparrow}^\dagger \tilde{c}_{\vec{r}_j, \downarrow}^\dagger & \tilde{n}_{\vec{r}_j, \uparrow} \tilde{n}_{\vec{r}_j, \downarrow} & -\tilde{c}_{\vec{r}_j, \downarrow}^\dagger \tilde{n}_{\vec{r}_j, \uparrow} & \tilde{c}_{\vec{r}_j, \uparrow}^\dagger \tilde{n}_{\vec{r}_j, \downarrow} \\ \tilde{c}_{\vec{r}_j, \uparrow}^\dagger (1 - \tilde{n}_{\vec{r}_j, \downarrow}) & -\tilde{n}_{\vec{r}_j, \uparrow} \tilde{c}_{\vec{r}_j, \downarrow}^\dagger & \tilde{n}_{\vec{r}_j, \uparrow} (1 - \tilde{n}_{\vec{r}_j, \downarrow}) & \tilde{c}_{\vec{r}_j, \uparrow}^\dagger \tilde{c}_{\vec{r}_j, \downarrow} \\ \tilde{c}_{\vec{r}_j, \downarrow}^\dagger (1 - \tilde{n}_{\vec{r}_j, \uparrow}) & \tilde{n}_{\vec{r}_j, \downarrow} \tilde{c}_{\vec{r}_j, \uparrow}^\dagger & \tilde{c}_{\vec{r}_j, \downarrow}^\dagger \tilde{c}_{\vec{r}_j, \uparrow} & \tilde{n}_{\vec{r}_j, \downarrow} (1 - \tilde{n}_{\vec{r}_j, \uparrow}) \end{bmatrix}. \quad (13)$$

As described in Ref.<sup>12</sup> for the polynomial  $\hat{O}_{\vec{r}_j}$ , one can as well introduce a general polynomial operator  $\tilde{O}_{\vec{r}_j}$  of rotated-electron operators of the general form,

$$\tilde{O}_{\vec{r}_j} = \sum_{l, l'} o_{\vec{r}_j, l, l'} \tilde{m}_{\vec{r}_j, l, l'} \equiv \text{Tr}(o_{\vec{r}_j} \tilde{m}_{\vec{r}_j}). \quad (14)$$

Lifting the local  $\eta$ -spin and spin  $SU(2) \times SU(2)$  gauge symmetry of the Hubbard model on a bipartite lattice for  $U/4t = \pm\infty$  to a global  $[SU(2) \times SU(2)]/Z_2 = SO(4)$  symmetry of that model for  $U/4t \neq 0$  is simply accomplished by summing over the  $N_a^D$  sites the six local generators  $\hat{O}_{\vec{r}_j}$  of the  $SU(2) \times SU(2)$  sub-group of the  $SU(2) \times SU(2) \times U(1)$  Lie group. It follows from the equalities of Eq. (11) that the six generators given in that equation can be represented by polynomials of electron and rotated-electron operators of the same form,  $\sum_{j=1}^{N_a^D} \hat{O}_{\vec{r}_j} = \sum_{j=1}^{N_a^D} \tilde{O}_{\vec{r}_j}$ . This holds in spite of except for  $U/4t \rightarrow \pm\infty$  the corresponding local generators  $\hat{O}_{\vec{r}_j}$  and  $\tilde{O}_{\vec{r}_j}$  being different operators,  $\hat{O}_{\vec{r}_j} \neq \tilde{O}_{\vec{r}_j}$ . Indeed, the local generators  $\hat{O}_{\vec{r}_j}$  do not in general commute with the unitary operator  $\hat{V}$ . This follows from  $\hat{m}_{\vec{r}_j, l'} \neq \tilde{m}_{\vec{r}_j, l'}$ , where  $\hat{m}_{\vec{r}_j, l'}$  and  $\tilde{m}_{\vec{r}_j, l'}$  appear in the expressions  $\hat{O}_{\vec{r}_j} = \sum_{l, l'} o_{\vec{r}_j, l, l'} \hat{m}_{\vec{r}_j, l} \equiv \text{Tr}(o_{\vec{r}_j} \hat{m}_{\vec{r}_j})$  and (14) of  $\tilde{O}_{\vec{r}_j}$ , respectively. However, the matrix  $o_{\vec{r}_j}$  appearing in these two expressions is the same. For the six local generators associated with the generators (11) of the global  $SO(4)$  symmetry it reads,

$$o_{\vec{r}_j} = \begin{bmatrix} -1/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}; \quad o_{\vec{r}_j} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & 1/2 \end{bmatrix} \quad (15)$$

for the  $\eta$ -spin and spin diagonal generators and

$$o_{\vec{r}_j} = \begin{bmatrix} 0 & -e^{i\vec{\pi} \cdot \vec{r}_j} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}; \quad o_{\vec{r}_j} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad (16)$$

plus their two hermitian conjugates for the  $\eta$ -spin and spin off-diagonal generators.

Now for the “rotated” Hamiltonian  $\tilde{H} = \hat{V}^\dagger \hat{H} \hat{V} = \tilde{V}^\dagger \hat{H} \tilde{V}$  a local  $SU(2) \times SU(2) \times U(1)$  gauge symmetry occurs for  $U/4t \rightarrow \pm\infty$  as well. Alike the original Hamiltonian,  $\tilde{H}$  has a global  $SO(4)$  symmetry whose generators are obtained as above. In addition, a similar procedure can be used to lift the local  $U(1)$  gauge symmetry to a global symmetry of the “rotated” Hamiltonian for  $t > 0$  and  $U/4t \neq 0$ . Indeed, through the polynomial of rotated-electron operators given in Eq. (14), the local generator of the “nonlinear” local  $U(1)$  gauge symmetry can be represented by a  $4 \times 4$  matrix given by,

$$o_{\vec{r}_j} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 \end{bmatrix}. \quad (17)$$

This local generator refers to rotated-electron single occupancy  $2S_c$ . The use of such a matrix  $o_{\vec{r}_j}$  in the polynomial  $\tilde{O}_{\vec{r}_j}$  of Eq. (14) leads for  $U/4t \neq 0$  to a sum of polynomials  $\sum_{j=1}^{N_a^D} \tilde{O}_{\vec{r}_j}$ . It exactly equals expression (8) of the generator of the global  $U(1)$  symmetry whose eigenvalue  $S_c$  is one half the number of rotated-electron singly occupied sites  $2S_c$ . The trivially related operator  $\tilde{S}_c^h \equiv [\tilde{D} + \tilde{D}^h]/2$  of eigenvalue  $S_c^h = [N_a^D/2 - S_c]$  can also generate such a global symmetry of the “rotated” Hamiltonian  $\tilde{H} = \hat{V}^\dagger \hat{H} \hat{V} = \tilde{V}^\dagger \hat{H} \tilde{V}$ . When written in terms of local polynomials as  $\sum_{j=1}^{N_a^D} \tilde{O}_{\vec{r}_j}$ , its corresponding matrix  $o_{\vec{r}_j}$  reads,

$$o_{\vec{r}_j} = \begin{bmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \quad (18)$$

This generator refers to rotated-electron double occupancy plus non occupancy  $[2N_a^D - 2S_c]$ . However,  $[2N_a^D - 2S_c]$  and rotated-electron single occupancy  $2S_c$  are not independent. Hence the operators  $\tilde{S}_c \equiv \tilde{Q}/2$  of Eq. (8) associated with the matrix  $o_{\vec{r}_j}$  of Eq. (17) and  $\tilde{S}_c^h \equiv [\tilde{D} + \tilde{D}^h]/2$  associated with the matrix  $o_{\vec{r}_j}$  of Eq. (18) refer to two alternative representations of the generator of the global  $U(1)$  symmetry of the “rotated” Hamiltonian under consideration.

The main point is that a global  $U(1)$  symmetry in the “rotated” Hamiltonian  $\tilde{H} = \hat{V}^\dagger \hat{H} \hat{V} = \tilde{V}^\dagger \hat{H} \tilde{V}$  for  $t > 0$  and  $U/4t \neq 0$  must also be a global  $U(1)$  symmetry, which is *hidden* in the original model  $\hat{H} = \hat{V} \tilde{H} \hat{V}^\dagger = \tilde{V} \tilde{H} \tilde{V}^\dagger$  of Eq. (7). Indeed, for the latter original model the generator (8) refers to one half the number of rotated electrons rather than electrons. And in contrast to the six generators (11) of the global  $SO(4)$  symmetry, the number of rotated electrons operator does not commute with the unitary operator  $\hat{V}$ . Other related operators  $\tilde{D}$ ,  $\tilde{D}^h$ , and  $\tilde{Q}_\sigma$ , which for

$U/4t \neq 0$  also commute with the Hamiltonian (1) yet do not commute with  $\hat{V}$ , are obtained by rotating the number operators  $\hat{D}$ ,  $\hat{D}^h$ , and  $\hat{Q}_\sigma$ , respectively, given in Eq. (3). For the  $N_a^D$ -site problem only for rotated electrons does single and double occupancy remain good quantum numbers for finite  $|U/4t| > 0$ , whereas for electrons single and double occupancy are conserved only for  $|U/4t| \rightarrow \infty$ . This is why the generator (8) does not commute with  $\hat{V}$ .

Since  $N_a^D$  is even, both  $[S_\eta + S_s^z]$  and  $[S_\eta^z + S_s^z]$  are integers. Their relation to  $S_c$  is such that  $2S_c$  and  $[N_a^D - 2S_c]$  give the number of spin-1/2 spins of the rotated electrons that singly occupy sites and the number of  $\eta$ -spin-1/2 " $\eta$ -spins", respectively. The former number equals that of rotated-electron singly occupied sites and the latter number that of rotated-electron doubly occupied sites (down  $\eta$ -spins) plus rotated-electron unoccupied sites (up  $\eta$ -spins), respectively. Therefore,  $[S_\eta^z + S_s^z + S_c]$  must also be an integer. This justifies why for  $U/4t \neq 0$  the global symmetry of the model (1) on a bipartite lattice is that of the group  $[SU(2) \times SU(2) \times U(1)]/Z_2^2 = SO(3) \times SO(3) \times U(1)$  rather than  $SU(2) \times SU(2) \times U(1)$ . The global  $U(1)$  symmetry remained hidden because in contrast to the six generators (11), one has that the generator  $\tilde{S}_c = \sum_{j=1}^{N_a^D} \tilde{O}_{\vec{r}_j}$  is except for  $|U/4t| \rightarrow \infty$  different from the operator  $\sum_{j=1}^{N_a^D} \hat{O}_{\vec{r}_j}$ . (Note that the matrix  $o_{\vec{r}_j}$  is given by Eq. (17) both in the  $\tilde{O}_{\vec{r}_j}$  and  $\hat{O}_{\vec{r}_j}$  expressions.) Indeed, when written in terms of electron creation and annihilation operators the expression of the generator  $\tilde{S}_c$  is for  $|U/4t|$  finite involved, consisting of an infinite number of operator terms,

$$\tilde{S}_c = \sum_{j=1}^{N_a^D} \hat{V}^\dagger \hat{O}_{\vec{r}_j} \hat{V} = \sum_{j=1}^{N_a^D} \left( \hat{O}_{\vec{r}_j} + [\hat{O}_{\vec{r}_j}, \hat{S}^\dagger] + \frac{1}{2} [[\hat{O}_{\vec{r}_j}, \hat{S}^\dagger], \hat{S}^\dagger] + \dots \right), \quad (19)$$

rather than merely by  $\sum_{j=1}^{N_a^D} \hat{O}_{\vec{r}_j}$ . Only for  $|U/4t| \rightarrow \infty$  one has that the commutator  $[\hat{O}_{\vec{r}_j}, \hat{S}^\dagger] = 0$  vanishes, so that  $\tilde{S}_c = \hat{S}_c = \sum_{j=1}^{N_a^D} \hat{O}_{\vec{r}_j}$ .

## B. Consistency between the global symmetry and the Hilbert space dimension

Addition of chemical-potential and magnetic-field operator terms to the Hamiltonian (1) lowers its symmetry. However, such terms commute with it. Therefore, the global symmetry being  $[SU(2) \times SU(2) \times U(1)]/Z_2^2 = SO(3) \times SO(3) \times U(1)$  implies that the set of independent rotated-electron occupancy configurations that generate the model energy eigenstates generate state representations of that global symmetry for all values of the electronic density  $n$  and spin density  $m$ . It then follows that the total number of such independent representations must equal the Hilbert-space dimension  $4^{N_a^D}$ . Here we show that for the Hubbard model on a bipartite lattice the number of independent representations of the group  $SO(3) \times SO(3) \times U(1)$  is indeed  $4^{N_a^D}$ . In contrast, the number of independent representations of the group  $SO(4)$  is for that model found to be smaller than its Hilbert-space dimension  $4^{N_a^D}$ . This is then consistent with the global symmetry of the Hubbard model on a bipartite lattice being larger than  $SO(4)$  and given by  $SO(3) \times SO(3) \times U(1)$ .

The rotated-electron occupancy configurations involving the (i) singly occupied and (ii) unoccupied and doubly-occupied sites are independent. They refer to the state representations of the spin  $SU(2)$  symmetry  $M_s = 2S_c$  spin-1/2 spins and  $\eta$ -spin  $SU(2)$  symmetry  $M_\eta = 2S_c^h$   $\eta$ -spin-1/2  $\eta$ -spins, respectively. Indeed, concerning the  $\eta$ -spin  $SU(2)$  representations the rotated-electron doubly occupied sites and unoccupied sites play the role of down and up  $\eta$ -spin-1/2  $\eta$ -spins, respectively. In turn, the  $U(1)$  symmetry state representations refer to the relative occupancy configurations of the  $2S_c$  rotated-electron singly-occupied sites and  $2S_c^h$  rotated-electron unoccupied and doubly-occupied sites. For  $U/4t \neq 0$ , the Hilbert space can then be divided into a set of subspaces with fixed  $S_\eta$ ,  $S_s$ , and  $S_c$  values and thus with the same values  $M_\eta = 2S_c^h$  of  $\eta$ -spins and  $M_s = 2S_c$  of spins. The number of  $SU(2) \times SU(2)$  state representations with both fixed values of  $S_\eta$  and  $S_s$ , which one can generate from  $M_\eta$   $\eta$ -spin-1/2  $\eta$ -spins and  $M_s$  spin-1/2 spins, reads  $\mathcal{N}(S_\eta, M_\eta) \cdot \mathcal{N}(S_s, M_s)$ . Here,

$$\mathcal{N}(S_\alpha, M_\alpha) = (2S_\alpha + 1) \left\{ \binom{M_\alpha}{M_\alpha/2 - S_\alpha} - \binom{M_\alpha}{M_\alpha/2 - S_\alpha - 1} \right\}, \quad (20)$$

for  $\alpha = \eta, s$ . If for  $U/4t \neq 0$  the global symmetry of the model was  $SO(4)$ , then the dimension of such a subspace would be  $\mathcal{N}(S_\eta, M_\eta) \cdot \mathcal{N}(S_s, M_s)$  and the sum of all sub-space dimensions would give the Hilbert-space dimension

$4^{N_a^D}$ . However, we confirm below that such a sum obeys the inequality,

$$\begin{aligned} & \sum_{M_s=0}^{N_a^D} \sum_{S_\eta=0}^{M_\eta/2} \sum_{S_s=0}^{M_s/2} \prod_{\alpha=\eta,s} \frac{[1 - (-1)^{2S_\alpha - (M_\eta - M_s)/2}]}{2} \mathcal{N}(S_\alpha, M_\alpha) \\ &= \sum_{M_\eta=0}^{N_a^D} \sum_{S_\eta=0}^{M_\eta/2} \sum_{S_s=0}^{M_s/2} \prod_{\alpha=\eta,s} \frac{[1 - (-1)^{2S_\alpha - (M_\eta - M_s)/2}]}{2} \mathcal{N}(S_\alpha, M_\alpha) < 4^{N_a^D}, \end{aligned} \quad (21)$$

and thus corresponds to a dimension smaller than  $4^{N_a^D}$ . Note that  $M_\eta = [N_a^D - M_s]$  so that the numbers  $M_\eta$  and  $M_s$  are not independent. Therefore, the sums over  $M_s = 0, 1, \dots, N_a^D$  and  $M_\eta = 0, 1, \dots, N_a^D$  are indeed alternative, as given in Eq. (21).

In turn, that the model global symmetry is larger than  $SO(4) = [SU(2) \times SU(2)]/Z_2$  and given by  $SO(3) \times SO(3) \times U(1) = [SU(2) \times SU(2) \times U(1)]/Z_2^2$  requires that one accounts for the number of representation states of the extra global  $U(1)$  symmetry. For  $U/4t \neq 0$  it has in the subspaces considered here,

$$d_c = \binom{N_a^D}{2S_c} = \binom{N_a^D}{2S_c^h}, \quad (22)$$

representation states. Thus rather than  $\mathcal{N}(S_\eta, M_\eta) \cdot \mathcal{N}(S_s, M_s)$  each of such subspaces has a larger dimension,

$$d(S_\eta, S_s, S_c) = d_c \cdot \mathcal{N}(S_\eta, N_a^D - 2S_c) \cdot \mathcal{N}(S_s, 2S_c). \quad (23)$$

By performing the sum over all subspaces, one then finds indeed in Appendix A that,

$$\begin{aligned} \mathcal{N}_{tot} &= \sum_{S_c=0}^{[N_a^D/2]} \sum_{S_\eta=0}^{[N_a^D/2 - S_c]} \sum_{S_s=0}^{S_c} \binom{N_a^D}{2S_c} \prod_{\alpha=\eta,s} \frac{[1 + (-1)^{2S_\alpha + 2S_c}]}{2} \mathcal{N}(S_\alpha, M_\alpha) = \sum_{S_\eta=0}^{[N_a^D/2]} \sum_{S_s=0}^{[N_a^D/2 - S_\eta]} \frac{[1 + (-1)^{2S_\eta + 2S_s}]}{2} \\ &\times (2S_\eta + 1)(2S_s + 1) \left[ \binom{N_a^D}{N_a^D/2 - S_\eta + S_s} \left\{ \binom{N_a^D}{N_a^D/2 - S_\eta - S_s} + \binom{N_a^D}{N_a^D/2 - S_\eta - S_s - 2} \right\} \right. \\ &\left. - \binom{N_a^D}{N_a^D/2 - S_\eta - S_s - 1} \left\{ \binom{N_a^D}{N_a^D/2 - S_\eta + S_s + 1} + \binom{N_a^D}{N_a^D/2 - S_\eta + S_s - 1} \right\} \right] = 4^{N_a^D}. \end{aligned} \quad (24)$$

Finally, except that a factor of one in each term of the two alternative sums of Eq. (21) is replaced by the dimension  $d_c$  in the sum of Eq. (24), such sums are identical. This is confirmed by transforming the sums over  $M_s = 0, 1, \dots, N_a^D$  and  $M_\eta = 0, 1, \dots, N_a^D$  of Eq. (21) in sums over  $S_c = M_s/2 = 0, 1/2, \dots, N_a^D/2$  and  $S_\eta = N_a^D/2 - M_\eta/2 = N_a^D/2, N_a^D/2 - 1/2, \dots, 1/2, 0$ , respectively, and accounting for that  $2S_c$  can be written as  $2S_c = N_a^D/2 - (M_\eta - M_s)/2$  where  $N_a^D/2$  is an odd integer number. That the dimension of Eq. (22) obeys the inequality  $d_c \geq 1$  then implies the validity of the inequality given in Eq. (21).

### C. Relation of the global symmetry to the exact solution of the 1D model

In the particular case of the bipartite 1D lattice the Hubbard model has an exact solution<sup>8–10</sup>. Since the global  $SO(3) \times SO(3) \times U(1)$  symmetry found here refers to 1D as well, it must be related to that exact solution. Such a solution refers to the 1D Hubbard model in the subspace spanned by the highest-weight states (HWSs) or lowest-weight states (LWSs) of both the  $\eta$ -spin  $SU(2)$  and spin  $SU(2)$  algebras. The model energy eigenstates that are HWSs or LWSs of these algebras are often called *Bethe states*. In order to clarify such a relation, rather than the so called coordinate Bethe ansatz<sup>8,9</sup>, it is convenient to consider the exact solution of the problem by the algebraic operator formulation of Ref.<sup>10</sup>. Within the latter formulation the HWSs or LWSs of the  $\eta$ -spin and spin algebras are built up in terms of linear combination of products of several types of annihilation or creation fields acting onto the hole or electronic vacuum, respectively.

The algebraic formulation of the Bethe states refers to the transfer matrix of the classical coupled spin model, which is the “covering” 1D Hubbard model<sup>15</sup>. Indeed, within the inverse scattering method<sup>10,16</sup> the central object to be diagonalized is the quantum transfer matrix rather than the underlying 1D Hubbard model. The transfer-matrix eigenvalues provide the spectrum of a set of conserved charges. The diagonalization of the charge degrees of

freedom involves a transfer matrix associated with a charge monodromy matrix of the form provided in Eq. (21) of Ref.<sup>10</sup>. Its off-diagonal entries are some of the creation and annihilation fields. The commutation relations of such important operators are given in Eqs. (25), (40)-(42), (B.1)-(B.3), (B.7)-(B.11), and (B.19)-(B.22) of that reference. The solution of the spin degrees of freedom involves the diagonalization of the auxiliary transfer matrix associated with the spin monodromy matrix provided in Eq. (95) of Ref.<sup>10</sup>. Again, the off-diagonal entries of that matrix play the role of creation and annihilation fields, whose commutation relations are given in Eq. (98) of that reference. The latter commutation relations correspond to the usual Faddeev-Zamolodchikov algebra associated with the traditional ABCD form of the elements of the monodromy matrix<sup>16</sup>. It also applies to the 1D isotropic Heisenberg model, whose global symmetry is  $SU(2)$ . Consistently, at half filling and for large  $U/4t$  values the latter model describes the spin degrees of freedom of the 1D Hubbard model. In turn, the above relations associated with the charge monodromy matrix refer to a different algebra. The corresponding form of that matrix is called ABCDF by the authors of Ref.<sup>10</sup>.

The main reason why the solution of the problem by the algebraic inverse scattering method<sup>10</sup> was achieved only thirty years after that of the coordinate Bethe ansatz<sup>8,9</sup> is that it was expected that the charge and spin monodromy matrices had the same traditional ABCD form, found previously for the related 1D isotropic Heisenberg model<sup>16</sup>. Indeed, such an expectation was that consistent with the occurrence of a spin  $SU(2)$  symmetry and a charge (and  $\eta$ -spin)  $SU(2)$  symmetry known long ago<sup>11</sup>, associated with a global  $SO(4) = [SU(2) \times SU(2)]/Z_2$  symmetry. If that was the whole global symmetry of the 1D Hubbard model, the charge and spin sectors would be associated with the  $\eta$ -spin  $SU(2)$  symmetry and spin  $SU(2)$  symmetry, respectively. A global  $SO(4) = [SU(2) \times SU(2)]/Z_2$  symmetry would then imply that the charge and spin monodromy matrices had indeed the same Faddeev-Zamolodchikov ABCD form.

However, all tentative schemes using charge and spin monodromy matrices of the same ABCD form failed to achieve the Bethe-ansatz equations obtained by means of the coordinate Bethe ansatz<sup>8,9</sup>. Fortunately, the problem was solved by Martins and Ramos, who used an appropriate representation of the charge and spin monodromy matrices, which allows for possible *hidden symmetries*<sup>10</sup>. Indeed, the structure of the charge and spin monodromy matrices introduced by these authors is able to distinguish creation and annihilation fields as well as possible hidden symmetries.

Our results refer to the Hubbard model on any bipartite lattice. Hence for the particular case of the bipartite 1D lattice they show that the hidden symmetry beyond  $SO(4)$  is the charge global  $U(1)$  symmetry found in this paper. Our studies reveal that for  $U/4t > 0$  the model charge and spin degrees of freedom are associated with  $U(2) = SU(2) \times U(1)$  and  $SU(2)$  symmetries, rather than with two  $SU(2)$  symmetries, respectively. The occurrence of such charge  $U(2) = SU(2) \times U(1)$  symmetry and spin  $SU(2)$  symmetry is behind the different ABCDF and ABCD forms of the charge and spin monodromy matrices of Eqs. (21) and (95) of Ref.<sup>10</sup>, respectively. Indeed, the former matrix is larger than the latter and involves more fields than expected from the model global  $SO(4) = [SU(2) \times SU(2)]/Z_2$  symmetry alone. This follows from the global symmetry of the model on the 1D and other bipartite lattices being  $SO(3) \times SO(3) \times U(1) = [SU(2) \times U(2)]/Z_2^2$  rather than  $SO(4) = [SU(2) \times SU(2)]/Z_2$ , as found in this paper. Hence our general results for the Hubbard model on a bipartite lattice are consistent with the algebraic operator formulation of its exact solution for the particular case of the 1D lattice<sup>10</sup>.

#### IV. CONCLUDING REMARKS

On a square lattice, the Hubbard model is one of the most studied condensed-matter quantum problems. Furthermore, on any bipartite lattice it is the simplest realistic toy model for description of the electronic correlation effects in general many-electron problems with short-range interaction. Therefore, that the global symmetry of the Hubbard model on a bipartite lattice is larger than  $SO(4)$  and given by  $SO(3) \times SO(3) \times U(1)$  is an important exact result in its own right. Furthermore, the new found global symmetry is expected to have important physical consequences.

The studies of Ref.<sup>17</sup> on the Hubbard model on the square lattice use a description in terms of quantum objects related to the rotated electrons. The introduction of such a description involves the global symmetry found in this paper and corresponding transformation laws under a suitable electron - rotated-electron unitary transformation of the type considered here and in Ref.<sup>13</sup>. The spinless  $c$  fermion, spin-1/2 spinon, and  $\eta$ -spin-1/2  $\eta$ -spinon operators of such a description are a generalization to  $U/4t > 0$  of the  $U/4t \gg 1$  “quasicharge”, spin, and “pseudospin” operators of Ref.<sup>14</sup>, respectively. The former quantum objects emerge from a suitable electron - rotated-electron unitary transformation. Their operators have the same expressions in terms of rotated-electron creation and annihilation operators as those of Ref.<sup>14</sup> in terms of electron creation and annihilation operators, respectively. The occupancy configurations of the spinless  $c$  fermions, spin-1/2 spinons, and  $\eta$ -spin-1/2  $\eta$ -spinons generate a set of complete states. Those correspond to representations of the  $U(1)$ , spin  $SU(2)$ , and  $\eta$ -spin  $SU(2)$  symmetries, respectively, associated with the three dimensions of Eq. (23) and the global symmetry found in this paper.

The square-lattice quantum liquid introduced in Ref.<sup>17</sup> contains the one- and two-electron excitations of the Hubbard model on a square lattice. At hole concentration  $x = [N_a^2 - N]/N_a^2 = 0$ ,  $U/4t \approx 1.525$ , and  $t \approx 295$  meV it is found



in that reference to quantitatively describing the spin-wave spectrum observed in the parent compound  $\text{La}_2\text{CuO}_4$ <sup>18</sup>. A system of weakly coupled planes, each described by the square-lattice quantum liquid of Ref.<sup>17</sup>, is the simplest realistic toy model for the description of the role of correlations effects in the unusual properties of the cuprate high-temperature superconductors<sup>5-7</sup>. After addition of such a weak three-dimensional uniaxial anisotropy perturbation, the Hamiltonian terms that describe the fluctuations of two important pairing phases are for intermediate  $U/4t$  values found to have the same general form as the microscopic Hamiltonian given in Eq. (1) of Ref.<sup>7</sup>. The main difference is that the electron creation and annihilation operators appear replaced by rotated-electron creation and annihilation operators, respectively. Evidence is provided elsewhere that such a quantum liquid has for a well-defined hole-concentration range a long-range superconducting order. In addition, it seems indeed to contain some of the microscopic mechanisms behind the unusual properties of the hole-doped cuprate high-temperature superconductors. It is commonly understood that Hamiltonian symmetries by themselves are not sufficient to prove that a particular symmetry is broken in the ground state. However, the symmetry of the action that describes the fluctuations of the phases of such a quantum liquid and of that of Ref.<sup>7</sup> is a global superconducting  $U(1)$  symmetry. In the case of the former quantum liquid the representations of such a  $U(1)$  symmetry are generated by  $c$  fermion occupancy configurations. Thus it is directly related to the original model hidden global  $U(1)$  symmetry found in this paper, whose representations are also generated by  $c$  fermion occupancy configurations. Such a preliminary result seems to confirm the important role plaid by the hidden  $U(1)$  symmetry of the global  $SO(3) \times SO(3) \times U(1)$  symmetry found in this paper for the Hubbard model on a bipartite lattice.

### Acknowledgments

We thank Alejandro Muramatsu, Tiago C. Ribeiro, and Pedro D. Sacramento for illuminating discussions, Tobias Stauber for calling our attention to Ref.<sup>13</sup> and for discussions, and the ESF Science programme INSTANS and the Portuguese PTDC/FIS/64926/2006 grant for support.

### Appendix A: Subspace-dimension summation

In this Appendix we perform the subspace-dimension summation of Eq. (24) that runs over  $S_c$ ,  $S_\eta$ , and  $S_s$  integer and half-odd-integer values. For simplicity here we consider the square lattice so that  $D = 2$  in Eq. (24), yet the derivation proceeds in a similar way for any other  $D$ -dimensional cubic lattice where  $D = 1, 2, 3, \dots$ . More generally, the sum-rule (24) is valid for the Hubbard model on any bipartite lattice. The subspace dimensions have the form  $d_r \cdot \prod_{\alpha=\eta,s} \mathcal{N}(S_\alpha, M_\alpha)$  given in Eq. (23) where  $\mathcal{N}(S_\alpha, M_\alpha)$  and  $d_r$  are provided in Eqs (20) and (22), respectively. Recounting the terms of Eq. (24), one may choose  $S_\eta$  to be the independent summation variable what gives,

$$\begin{aligned} \sum_{S_c=0}^{N_a^2/2} \sum_{S_\eta=0}^{[N_a^2/2-S_c]} \sum_{S_s=0}^{S_c} \frac{1 + (-1)^{2(S_\eta+S_c)}}{2} \frac{1 + (-1)^{2(S_s+S_c)}}{2} \dots = \\ = \sum_{S_\eta=0}^{N_a^2/2} \sum_{S_s=0}^{[\frac{N_a^2}{2}-S_\eta]} \sum_{S_c=S_s}^{[\frac{N_a^2}{2}-S_\eta]} \frac{1 + (-1)^{2(S_\eta+S_s)}}{2} \frac{1 + (-1)^{2(S_s+S_c)}}{2} \dots \end{aligned} \quad (\text{A1})$$

One can then rewrite the summation (24) in the form,

$$\mathcal{N}_{tot} = \sum_{S_\eta=0}^{N_a^2/2} \sum_{S_s=0}^{[N_a^2/2-S_\eta]} \frac{1 + (-1)^{2(S_\eta+S_s)}}{2} (2S_\eta + 1)(2S_s + 1) \times \Sigma(S_\eta, S_s), \quad (\text{A2})$$

where  $\Sigma(S_\eta, S_s)$  denotes the  $S_\eta$  and  $S_s$  dependent summation over  $S_c$  as follows,

$$\begin{aligned} \Sigma(S_\eta, S_s) = & \sum_{S_c=S_s}^{\frac{N_a^2}{2}-S_\eta} \frac{1+(-1)^{2(S_s+S_c)}}{2} \binom{N_a^2}{2S_c} \times \\ & \left[ \binom{N_a^2-2S_c}{\frac{N_a^2}{2}-S_c-S_\eta} - \binom{N_a^2-2S_c}{\frac{N_a^2}{2}-S_c-S_\eta-1} \right] \left[ \binom{2S_c}{S_c-S_s} - \binom{2S_c}{S_c-S_s-1} \right] \\ & \sum_{S_c=S_s}^{\frac{N_a^2}{2}-S_\eta} \frac{1+(-1)^{2(S_s+S_c)}}{2} N_a^2! \left[ \frac{1}{(S_c-S_s)!(S_c+S_s)!} - \frac{1}{(S_c-S_s-1)!(S_c+S_s+1)!} \right] \times \\ & \left[ \frac{1}{(N_a^2/2-S_c-S_\eta)!(N_a^2/2-S_c+S_\eta)!} - \frac{1}{(N_a^2/2-S_c-S_\eta-1)!(N_a^2/2-S_c+S_\eta+1)!} \right]. \quad (\text{A3}) \end{aligned}$$

In order to evaluate  $\Sigma(S_\eta, S_s)$  it is useful to replace the variable  $S_c$  by  $k = S_c - S_s$ . To simplify the notation we then introduce,

$$\mathcal{S} = S_\eta + S_s = \mathcal{S}(S_\eta, S_s); \quad \mathcal{D} = S_\eta - S_s = \mathcal{D}(S_\eta, S_s). \quad (\text{A4})$$

Due to the parity factor, in the summation over  $k$  only the terms with  $k$  integer survive so that,

$$\begin{aligned} \Sigma = & \sum_{k=0}^{\frac{N_a^2}{2}-\mathcal{S}} N_a^2! \left[ \frac{1}{k!(\mathcal{S}-\mathcal{D}+k)!} - \frac{1}{(k-1)!(\mathcal{S}-\mathcal{D}+k+1)!} \right] \times \\ & \left[ \frac{1}{(N_a^2/2-\mathcal{S}-k)!(N_a^2/2+\mathcal{D}-k)!} - \frac{1}{(N_a^2/2-\mathcal{S}-k-1)!(N_a^2/2+\mathcal{D}-k+1)!} \right] \\ = & \sum_{k=0}^{\frac{N_a^2}{2}-\mathcal{S}} N_a^2! \left\{ \frac{1}{k!(\mathcal{S}-\mathcal{D}+k)!} \frac{1}{(N_a^2/2-\mathcal{S}-k)!(N_a^2/2+\mathcal{D}-k)!} - \right. \\ & - \frac{1}{k!(\mathcal{S}-\mathcal{D}+k)!} \frac{1}{(N_a^2/2-\mathcal{S}-k-1)!(N_a^2/2+\mathcal{D}-k+1)!} - \\ & - \frac{1}{(k-1)!(\mathcal{S}-\mathcal{D}+k+1)!} \frac{1}{(N_a^2/2-\mathcal{S}-k)!(N_a^2/2+\mathcal{D}-k)!} + \\ & \left. + \frac{1}{(k-1)!(\mathcal{S}-\mathcal{D}+k+1)!} \frac{1}{(N_a^2/2-\mathcal{S}-k-1)!(N_a^2/2+\mathcal{D}-k+1)!} \right\}, \quad (\text{A5}) \end{aligned}$$

where now the  $k$  summation runs over integers only.

In order to perform the summation (A5) we rearrange the terms as follows,

$$\begin{aligned} \Sigma = & \sum_{k=0}^{\frac{N_a^2}{2}-\mathcal{S}} \left\{ \frac{1}{(N_a^2/2+\mathcal{D})!(N_a^2/2-\mathcal{D})!} \left[ \binom{N_a^2/2+\mathcal{D}}{k} \binom{N_a^2/2-\mathcal{D}}{N_a^2/2-\mathcal{S}-k} + \binom{N_a^2/2+\mathcal{D}}{k-1} \binom{N_a^2/2-\mathcal{D}}{N_a^2/2-\mathcal{S}-k-1} \right] - \right. \\ & - \frac{1}{(N_a^2/2+\mathcal{D}+1)!(N_a^2/2-\mathcal{D}-1)!} \binom{N_a^2/2+\mathcal{D}+1}{k} \binom{N_a^2/2-\mathcal{D}-1}{N_a^2/2-\mathcal{S}-k-1} - \\ & \left. - \frac{1}{(N_a^2/2+\mathcal{D}-1)!(N_a^2/2-\mathcal{D}+1)!} \binom{N_a^2/2+\mathcal{D}-1}{k-1} \binom{N_a^2/2-\mathcal{D}+1}{N_a^2/2-\mathcal{S}-k} \right\} N_a^2!, \quad (\text{A6}) \end{aligned}$$

or

$$\begin{aligned}
\Sigma = & \binom{N_a^2}{N_a^2/2 - \mathcal{D}} \sum_{k=0}^{\frac{N_a^2}{2} - \mathcal{S}} \left[ \binom{N_a^2/2 + \mathcal{D}}{k} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k} + \binom{N_a^2/2 + \mathcal{D}}{k-1} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k - 1} \right] - \\
& - \binom{N_a^2}{N_a^2/2 - \mathcal{D} - 1} \sum_{k=0}^{\frac{N_a^2}{2} - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D} + 1}{k} \binom{N_a^2/2 - \mathcal{D} - 1}{N_a^2/2 - \mathcal{S} - k - 1} - \\
& - \binom{N_a^2}{N_a^2/2 - \mathcal{D} + 1} \sum_{k=0}^{\frac{N_a^2}{2} - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D} - 1}{k-1} \binom{N_a^2/2 - \mathcal{D} + 1}{N_a^2/2 - \mathcal{S} - k}.
\end{aligned} \tag{A7}$$

Next, by using the identity,

$$\sum_{k=0}^N \binom{A}{k} \binom{B}{N-k} = \binom{A+B}{N}, \tag{A8}$$

we carry out separately the summations in expression (A7), what gives,

$$\sum_{k=0}^{N_a^2/2 - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D}}{k} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k} = \binom{N_a^2}{N_a^2/2 - \mathcal{S}}, \tag{A9}$$

$$\begin{aligned}
\sum_{k=0}^{N_a^2/2 - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D}}{k-1} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k - 1} &= \sum_{k=1}^{N_a^2/2 - \mathcal{S} - 1} \binom{N_a^2/2 + \mathcal{D}}{k-1} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k - 1} \\
&= \sum_{k'=0}^{N_a^2/2 - \mathcal{S} - 2} \binom{N_a^2/2 + \mathcal{D}}{k'} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - 2 - k'} \\
&= \binom{N_a^2}{N_a^2/2 - \mathcal{S} - 2},
\end{aligned} \tag{A10}$$

$$\begin{aligned}
\sum_{k=0}^{N_a^2/2 - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D} + 1}{k} \binom{N_a^2/2 - \mathcal{D} - 1}{N_a^2/2 - \mathcal{S} - k - 1} &= \sum_{k=0}^{N_a^2/2 - \mathcal{S} - 1} \binom{N_a^2/2 + \mathcal{D} + 1}{k} \binom{N_a^2/2 - \mathcal{D} - 1}{N_a^2/2 - \mathcal{S} - 1 - k} \\
&= \binom{N_a^2}{N_a^2/2 - \mathcal{S} - 1},
\end{aligned} \tag{A11}$$

and

$$\begin{aligned}
\sum_{k=0}^{N_a^2/2 - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D} - 1}{k-1} \binom{N_a^2/2 - \mathcal{D} + 1}{N_a^2/2 - \mathcal{S} - k} &= \sum_{k=1}^{N_a^2/2 - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D} - 1}{k-1} \binom{N_a^2/2 - \mathcal{D} + 1}{N_a^2/2 - \mathcal{S} - k} \\
&= \sum_{k'=0}^{N_a^2/2 - \mathcal{S} - 1} \binom{N_a^2/2 + \mathcal{D} - 1}{k'} \binom{N_a^2/2 - \mathcal{D} + 1}{N_a^2/2 - \mathcal{S} - 1 - k'} \\
&= \binom{N_a^2}{N_a^2/2 - \mathcal{S} - 1}.
\end{aligned} \tag{A12}$$

Introducing these results in expression (A7) for  $\Sigma$  leads to,

$$\begin{aligned}
\Sigma(S_\eta, S_s) &= \binom{N_a^2}{N_a^2/2 - \mathcal{D}} \left[ \binom{N_a^2}{N_a^2/2 - \mathcal{S}} + \binom{N_a^2}{N_a^2/2 - \mathcal{S} - 2} \right] - \\
&\quad - \binom{N_a^2}{N_a^2/2 - \mathcal{S} - 1} \left[ \binom{N_a^2}{N_a^2/2 - \mathcal{D} + 1} + \binom{N_a^2}{N_a^2/2 - \mathcal{D} - 1} \right] \\
&\equiv \Sigma(\mathcal{S}, \mathcal{D}).
\end{aligned} \tag{A13}$$

Expression (A2) for  $\mathcal{N}_{tot}$  can now be rewritten as,

$$\begin{aligned} \mathcal{N}_{tot} = & \sum_{S_\eta=0}^{N_a^2/2} \sum_{S_s=0}^{[N_a^2/2-S_\eta]} \frac{1+(-1)^{2(S_\eta+S_s)}}{2} (2S_\eta+1)(2S_s+1) \times \\ & \left\{ \binom{N_a^2}{N_a^2/2-(S_\eta-S_s)} \left[ \binom{N_a^2}{N_a^2/2-(S_\eta+S_s)} + \binom{N_a^2}{N_a^2/2-(S_\eta+S_s)-2} \right] - \right. \\ & \left. - \binom{N_a^2}{N_a^2/2-(S_\eta+S_s)-1} \left[ \binom{N_a^2}{N_a^2/2-(S_\eta-S_s)+1} + \binom{N_a^2}{N_a^2/2-(S_\eta-S_s)-1} \right] \right\}, \end{aligned} \quad (\text{A14})$$

where the summations run over both integers and half-odd integers. The use of the notation (A4) then allows rewriting (A14) in compact form,

$$\mathcal{N}_{tot} = \sum_{S_\eta=0}^{N_a^2/2} \sum_{S_s=0}^{[N_a^2/2-S_\eta]} \frac{1+(-1)^{2S}}{2} (S+\mathcal{D}+1)(S-\mathcal{D}+1) \times \Sigma(\mathcal{S}, \mathcal{D}), \quad (\text{A15})$$

where the summations run again over both integers and half-odd integers.

We can perform the summations of Eq. (A15) in the integers  $\mathcal{S}$  and  $\mathcal{D}$  instead of in  $S_\eta$  and  $S_s$ . Indeed, the first factor cancels all the terms with  $\mathcal{S}$  and  $\mathcal{D}$  non-integer so that,

$$\begin{aligned} \sum_{S_\eta=0}^{N_a^2/2} \sum_{S_s=0}^{[N_a^2/2-S_\eta]} \frac{1+(-1)^{2(S_\eta+S_s)}}{2} \cdots (S_\eta \text{ and } S_s \text{ both either integers or half odd integers}) = \\ = \sum_{S=0}^{N_a^2/2} \sum_{\mathcal{D}=-S}^{+\mathcal{S}} \cdots (\mathcal{S} \text{ and } \mathcal{D} \text{ integers}). \end{aligned}$$

Thus we find,

$$\mathcal{N}_{tot} = \sum_{S=0}^{N_a^2/2} \sum_{\mathcal{D}=-S}^{+\mathcal{S}} ((S+1)^2 - \mathcal{D}^2) \times \Sigma(\mathcal{S}, \mathcal{D}).$$

The use of the result (A13) then leads to,

$$\begin{aligned} \mathcal{N}_{tot} = \sum_{S=0}^{N_a^2/2} \sum_{\mathcal{D}=-S}^S ((S+1)^2 - \mathcal{D}^2) \left\{ \binom{N_a^2}{N_a^2/2-\mathcal{D}} \left[ \binom{N_a^2}{N_a^2/2-S} + \binom{N_a^2}{N_a^2/2-S-2} \right] - \right. \\ \left. - \binom{N_a^2}{N_a^2/2-S-1} \left[ \binom{N_a^2}{N_a^2/2-\mathcal{D}+1} + \binom{N_a^2}{N_a^2/2-\mathcal{D}-1} \right] \right\}. \end{aligned} \quad (\text{A16})$$

Replacing the variable  $\mathcal{S}$  by  $\mathcal{S}' = \mathcal{S} + 1$  we reach a more tractable expression for  $\mathcal{N}_{tot}$ ,

$$\mathcal{N}_{tot} = \sum_{S'=1}^{N_a^2/2+1} \sum_{\mathcal{D}=-S'+1}^{S'-1} \mathcal{T}(S', \mathcal{D}), \quad (\text{A17})$$

where

$$\begin{aligned} \mathcal{T}(S', \mathcal{D}) &= ((S')^2 - \mathcal{D}^2) \times \Sigma(S'-1, \mathcal{D}) \\ &= (S'^2 - \mathcal{D}^2) \left\{ \binom{N_a^2}{N_a^2/2-\mathcal{D}} \left[ \binom{N_a^2}{N_a^2/2-S'+1} + \binom{N_a^2}{N_a^2/2-S'-1} \right] - \right. \\ &\quad \left. - \binom{N_a^2}{N_a^2/2-S'} \left[ \binom{N_a^2}{N_a^2/2-\mathcal{D}+1} + \binom{N_a^2}{N_a^2/2-\mathcal{D}-1} \right] \right\}, \end{aligned} \quad (\text{A18})$$

is completely symmetric in the summation variables.

Since  $\mathcal{T}(\mathcal{S}', \mathcal{D} = \pm \mathcal{S}') = 0$ , we can extend the summation over  $\mathcal{D}$  of Eq.(A17) to  $\mathcal{D} = \pm \mathcal{S}'$ . We then formally extend the summation over  $\mathcal{S}'$  to  $\mathcal{S}' = 0$  because the corresponding term vanishes:  $\mathcal{T}(\mathcal{S}' = 0, \mathcal{D} = 0) = 0$ . Furthermore,  $\mathcal{T}(\pm \mathcal{S}', \mathcal{D}) = \mathcal{T}(\mathcal{S}', \pm \mathcal{D}) = \mathcal{T}(\mathcal{S}', \mathcal{D})$ , and due to the symmetry  $\mathcal{S}' \leftrightarrow \mathcal{D}$  we can write,

$$\sum_{\mathcal{S}'=1}^{N_a^2/2} \sum_{\mathcal{D}=-\mathcal{S}'+1}^{\mathcal{S}'-1} \mathcal{T}(\mathcal{S}', \mathcal{D}) = \frac{1}{4} \sum_{\mathcal{S}', \mathcal{D}=-(N_a^2/2+1)}^{N_a^2/2+1} \mathcal{T}(\mathcal{S}', \mathcal{D}). \quad (\text{A19})$$

Let us introduce the numbers  $p$  and  $q$  such that,

$$\begin{aligned} \mathcal{S}' + N_a^2/2 + 1 &= p \Leftrightarrow \mathcal{S}' = p - (N_a^2/2 + 1) \\ \mathcal{D} + N_a^2/2 + 1 &= q \Leftrightarrow \mathcal{D} = q - (N_a^2/2 + 1). \end{aligned}$$

The use of (A19) then allows rewriting (A17) as,

$$\begin{aligned} \mathcal{N}_{tot} &= \frac{1}{4} \sum_{p,q=0}^{N_a^2+2} [q(N_a^2 + 2 - q) - p(N_a^2 + 2 - p)] \\ &\quad \times \left\{ \binom{N_a^2}{q-1} \left[ \binom{N_a^2}{p} + \binom{N_a^2}{p-2} \right] - \binom{N_a^2}{p-1} \left[ \binom{N_a^2}{q} + \binom{N_a^2}{q-2} \right] \right\}. \end{aligned} \quad (\text{A20})$$

This expression can be simplified noticing that,

$$\binom{N}{x} + \binom{N}{x-2} = -2 \binom{N}{x-1} + \binom{N+2}{x}.$$

Replacing in Eq.(A20) one then finds,

$$\begin{aligned} \mathcal{N}_{tot} &= \frac{1}{4} \sum_{p,q=0}^{N_a^2+2} \left[ q(N_a^2 + 2 - q) - p(N_a^2 + 2 - p) \right] \left\{ \binom{N_a^2}{q-1} \binom{N_a^2+2}{p} - \binom{N_a^2}{p-1} \binom{N_a^2+2}{q} \right\} \\ &= \frac{1}{4} \sum_{p,q=0}^{N_a^2+2} \left\{ q(N_a^2 + 2 - q) \left[ \binom{N_a^2}{q-1} \binom{N_a^2+2}{p} - \binom{N_a^2}{p-1} \binom{N_a^2+2}{q} \right] + (q \leftrightarrow p) \right\} \\ &= \frac{1}{4} 2 \left\{ \sum_{q=0}^{N_a^2+2} q(N_a^2 + 2 - q) \binom{N_a^2}{q-1} \sum_{p=0}^{N_a^2+2} \binom{N_a^2+2}{p} - \sum_{q=0}^{N_a^2+2} q(N_a^2 + 2 - q) \binom{N_a^2}{q} \sum_{p=0}^{N_a^2+2} \binom{N_a^2}{p-1} \right\}. \end{aligned} \quad (\text{A21})$$

Finally, the use of the identities,

$$\begin{aligned} \sum_{k=0}^N \binom{N}{k} &= 2^N, \\ \sum_{k=0}^{N+2} \binom{N}{k-1} &= \sum_{k=1}^{N+1} \binom{N}{k-1} = \sum_{k'=0}^N \binom{N}{k'} = 2^N, \\ \sum_{k=0}^N k(N-k) \binom{N}{k} &= \sum_{k=1}^{N-1} \frac{N!}{(k-1)!(N-k-1)!} = N(N-1) \sum_{k=1}^{N-2} \binom{N-2}{k-1} \\ &= N(N-1) 2^{N-2}, \end{aligned}$$

and

$$\begin{aligned} \sum_{k=0}^{N+2} k(N+2-k) \binom{N}{k-1} &= \sum_{k=1}^{N+1} k(N+2-k) \binom{N}{k-1} = \sum_{k=1}^N k(N+2-k) \binom{N}{k-1} \\ &= \sum_{k'=0}^N (k'+1)(N-k'+1) \binom{N}{k'} = \sum_{k'=0}^N [k'(N-k') + (N+1)] \binom{N}{k'} \\ &= N(N-1) 2^{N-2} + (N+1) 2^N = 2^{N-2} [N(N-1) + 4(N+1)] \\ &= [N^2 + 3N + 4] 2^{N-2}, \end{aligned}$$

leads to,

$$\mathcal{N}_{tot} = \frac{1}{2} \left\{ [N_a^2 + 3N_a^2 + 4] 2^{N_a^2-2} \times 2^{N_a^2+2} - (N_a^2 + 2)(N_a^2 + 1) 2^{N_a^2} \times 2^{N_a^2} \right\} = \frac{1}{2} 2^{2N_a^2} \times 2 = 4^{N_a^2}, \quad (\text{A22})$$

which is the desired result.

- 
- <sup>1</sup> D. Jaksch, P. Zoller, Ann. Phys. 315 (2005) 52.  
<sup>2</sup> R. Jördens, N. Strohmaier, K. Günter, H. Moritz, T. Esslinger, Nature 455 (2008) 204.  
<sup>3</sup> M. Sing, U. Schwingenschlögl, R. Claessen, P. Blaha, J. M. P. Carmelo, L. M. Martelo, P. D. Sacramento, M. Dressel, C. S. Jacobsen, Phys. Rev. B 68 (2003) 125111.  
<sup>4</sup> J. M. P. Carmelo, D. Bozi, K. Penc, J. Phys.: Cond. Matt. 20 (2008) 415103; D. Bozi, J. M. P. Carmelo, K. Penc, P. D. Sacramento, J. Phys.: Cond. Matt. 20 (2008) 022205.  
<sup>5</sup> A. Damascelli, Z. Hussain, Z.-X. Shen, Rev. Mod. Phys. 75 (2003) 473.  
<sup>6</sup> P. A. Lee, N. Nagaosa, X.-G. Wen, Rev. Mod. Phys. 78 (2006) 17.  
<sup>7</sup> Z. Tešanović, Nature Phys., 4 (2008) 408.  
<sup>8</sup> E. H. Lieb, F. Y. Wu, Phys. Rev. Lett. 20 (1968) 1445.  
<sup>9</sup> Minoru Takahashi, Progr. Theor. Phys 47 (1972) 69.  
<sup>10</sup> M. J. Martins, P. B. Ramos, Nucl. Phys. B 522 (1998) 413.  
<sup>11</sup> O. J. Heilmann, E. H. Lieb, Ann. N. Y. Acad. Sci. 172 (1971) 583; E. H. Lieb, Phys. Rev. Lett. 62 (1989) 1201; C. N. Yang, S. C. Zhang, Mod. Phys. Lett. B 4 (1990) 759; S. C. Zhang, Phys. Rev. Lett. 65 (1990) 120.  
<sup>12</sup> Stellan Östlund, Eugene Mele, Phys. Rev. B 44 (1991) 12413.  
<sup>13</sup> J. Stein, J. Stat. Phys. 88 (1997) 487.  
<sup>14</sup> Stellan Östlund, Mats Granath, Phys. Rev. Lett. 96 (2006) 066404.  
<sup>15</sup> B. Sriram Shastry, J. Stat. Phys. 50 (1988) 57.  
<sup>16</sup> E. K. Sklyanin, L. A. Takhtadzhian, L. D. Faddeev, Theor. Math. Fiz. 40 (1979) 194.  
<sup>17</sup> J. M. P. Carmelo, Nucl. Phys. B 824 (2010) 452 and references therein.  
<sup>18</sup> R. Coldea, S. M. Hayden, G. Aeppli, T. G. Perring, C. D. Frost, T. E. Mason, S.-W. Cheong, Z. Fisk, Phys. Rev. Lett. 86 (2001) 5377.